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# Simulation of Soil-Plant Nitrogen Interactions for Educational Purposes

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## ABSTRACT

**A computer model characterizing the balance of soil-plant N is described, which is coded in a language that provides a graphic interface for use by students and others with minimal programming experience. Equations representing simultaneous water, C, and N balance reactions in a soil-plant system are solved over time. Both qualitative and quantitative relationships between various interacting system components are presented in graphic form to facilitate an intuitive understanding of the dynamic interactions between system functions. By manipulating various combinations of input functions, the student can see the likely consequences of different biological and weather related parameters upon the N cycle. Three uses for the model are proposed: (i) orienting beginning students toward an understanding of fundamental components of the soil N cycle, (ii) providing in-depth information for advanced students including access to the defining equations and citations of relevant journal articles, and (iii) supplying source-equations for scientists who may wish to extend the model or explore the dynamic consequences of using alternate formulations.**

THE N cycle in the soil-plant system is a dynamic process with complex physical, biological, and chemical components. Understanding these different components and how they interact can be difficult, but it is important that students involved in agricultural and environmental sciences have a good understanding of these processes.

Much effort has been invested in developing computer programs to help scientists and others predict the fate of N in the environment. Tanji (1982) listed 21 references to N simulation models and their subsequent applications. These programs, however, are primarily aimed at making predictions about the fate of N for either scientific inquiry or grower decision-support. None of the computer programs presently available is intended to help students understand the dynamics of the N cycle itself. Programs such as those described by Tanji et al. (1981) or Slim and Iskandar (1981) are quite sophisticated, representing our best scientific understanding of the N cycle. The computer code that represents the workings of the N cycle, however, is usually programmed in computer languages that are rarely accessible or understandable by the general public.

Recent computer software developments such as the STELLA II[1] (or ithink) software for Macintosh[2] personal computers has facilitated a new approach to computer modeling of the N cycle. The interface between user and computer has been modified to mediate between the user and the main program, so that it is no longer necessary to be highly proficient in computer programming. These STELLA II programs allow graphic modeling of the internal relationships of complicated systems without an in-depth knowledge of computer languages. We developed a program using this software to help students understand the N cycle. A description of the model and its usage follows.

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## MATERIALS AND METHODS

### Model Description

The computer model represents chemical transformations of N under typical agricultural production systems (Fig. 1). The flow of N between various N pools is controlled by reaction components ($K_1 \ldots K_h$) using standard chemical reaction kinetic equations. The model is based on the *unit world* concept, with the unit world being 1 acre furrow-slice of soil (0.42 ha by 15 cm deep). The model is designed to follow daily changes in the various N pools over a time span of 1 yr. Climatic factors such as temperature and rainfall are also modeled to generate the interactive controls of these factors upon the N cycle. Soil moisture condition is measured as soil weight expressed as the sum of mineral, organic, and water components.

### Screen Display

The screen display uses diagram icons (Fig. 2) developed by the STELLA II computer program to schematically represent the process being modeled. Each constituent ($NH_4^+$, $NO_3^-$, organic N, etc.) is represented as a *stock* (rectangle). Each reaction rate (material flow between components) is represented as a *pipe* between the rectangles, with a *valve* to regulate the flow of material along each pipe. Material flow can only occur along pipes; therefore, material flow into or out of the system being modeled is accomplished by connecting a stock to a *cloud*. The clouds represent a method for introducing material from outside of the model into the model system or to remove material that is leaving the system. The diagrams also contain *converters* (circles) linked to the valves with *connectors* (single-line arrow), which represents the flow of information or a control function, but not material. The various constituents can be distinguished by their assigned names, written near each valve,

[1] From High Performance Systems, 45 Lyme Road, Hanover, NH 03755.

[2] Trade names supplied for the convenience of the reader; does not imply endorsement by the USDA or the University of Illinois.

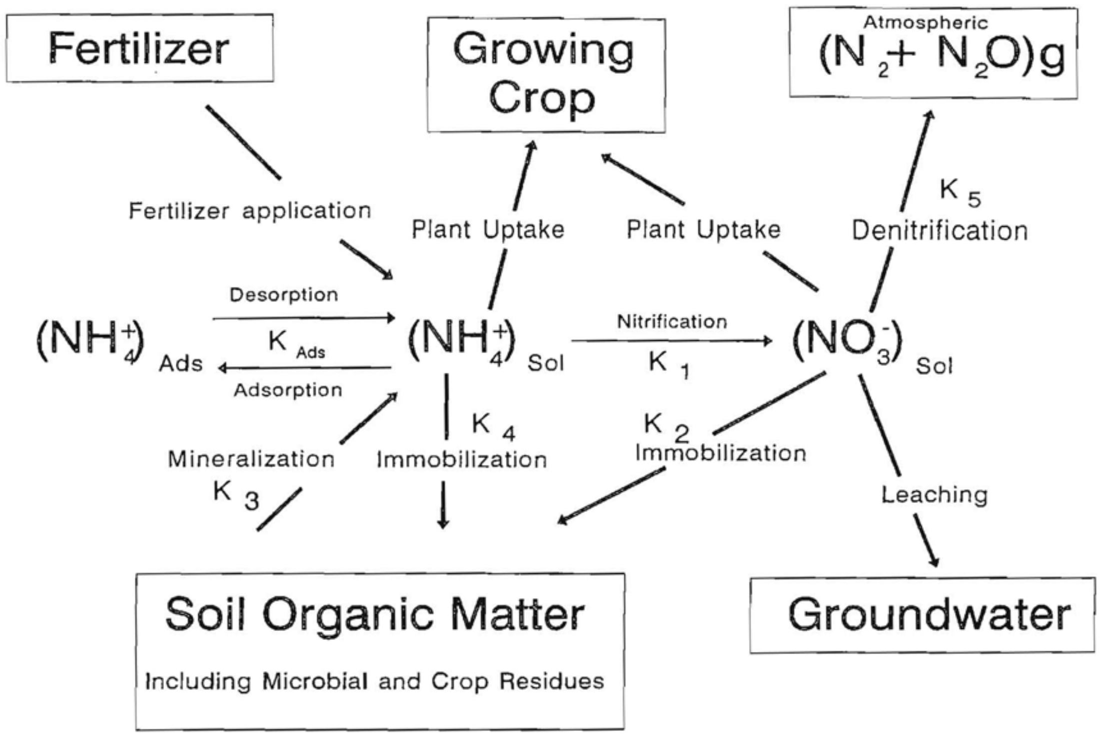


**Fig. 1. A general schematic of processes being considered by the simulation model, expressed as chemical reaction kinetic equations. Mass balance equilibrium constants represented by *K* values as indicated in text.**

converter, or stock. When the value of a stock or converter is needed in other portions of the model for calculations, the icons are drawn with dotted lines, or a *ghost*, meaning that this constituent was computed elsewhere in the model. (For a more thorough description see *STELLA II User's Guide*, Richmond et al., 1990.) Figure 3 is a typical example of the screen view found in the N model.

Literature citations from which each of the defining equations were derived are cited in the program as *comments* in the source code. Names written on the model icons correspond exactly to variable-names in the defining equations, which are based on theoretical or experimentally observed processes that have been described elsewhere in the scientific literature. Numerical values for each converter or stock are computed according to the defining equations at every time step as the simulation proceeds, from values assigned at initialization or by results from earlier calculations.

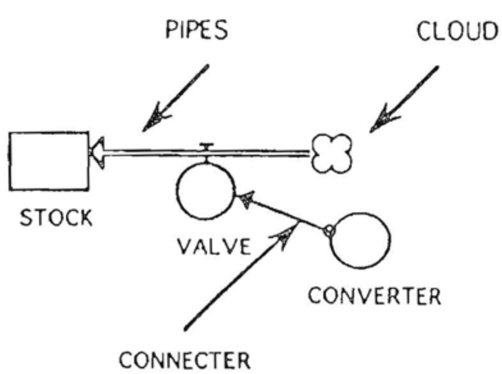


**Fig. 2. Model icons of a STELLA diagram. *Stocks* represent the actual quantity of a particular component at a given time. Flow of material occurs along *pipes*, and proceeds at a rate controlled by the *valves* shown adjacent to the *pipes*. Auxiliary variables used in the calculation of flow-rates are shown as converters with connectors to the *valves* whose rate they control.**

## RESULTS

### User Interaction

Because of its intuitive nature, our program can be useful at three levels of understanding: (i) *beginner*, (ii) *in-depth*, or (iii) *advanced*.

#### Beginner

At the beginner level, students having no prior knowledge of the N cycle (or only a rudimentary understanding) are required to understand only the processes and factors that interact in the N cycle. At this level, the student is presented with a series of six different choices that allow changing such environmental parameters as temperature and rainfall pattern and cultural practices such as planting date and fertilization. These choices generate different scenarios, so that the student can watch the effects (if any) of these changes on various components of the N cycle. Model results can be followed either graphically or numerical values tabulated in a window on the screen.

Use of the STELLA II software permits the user to operate a relatively complex network of simultaneous differential equations by entering parameter values

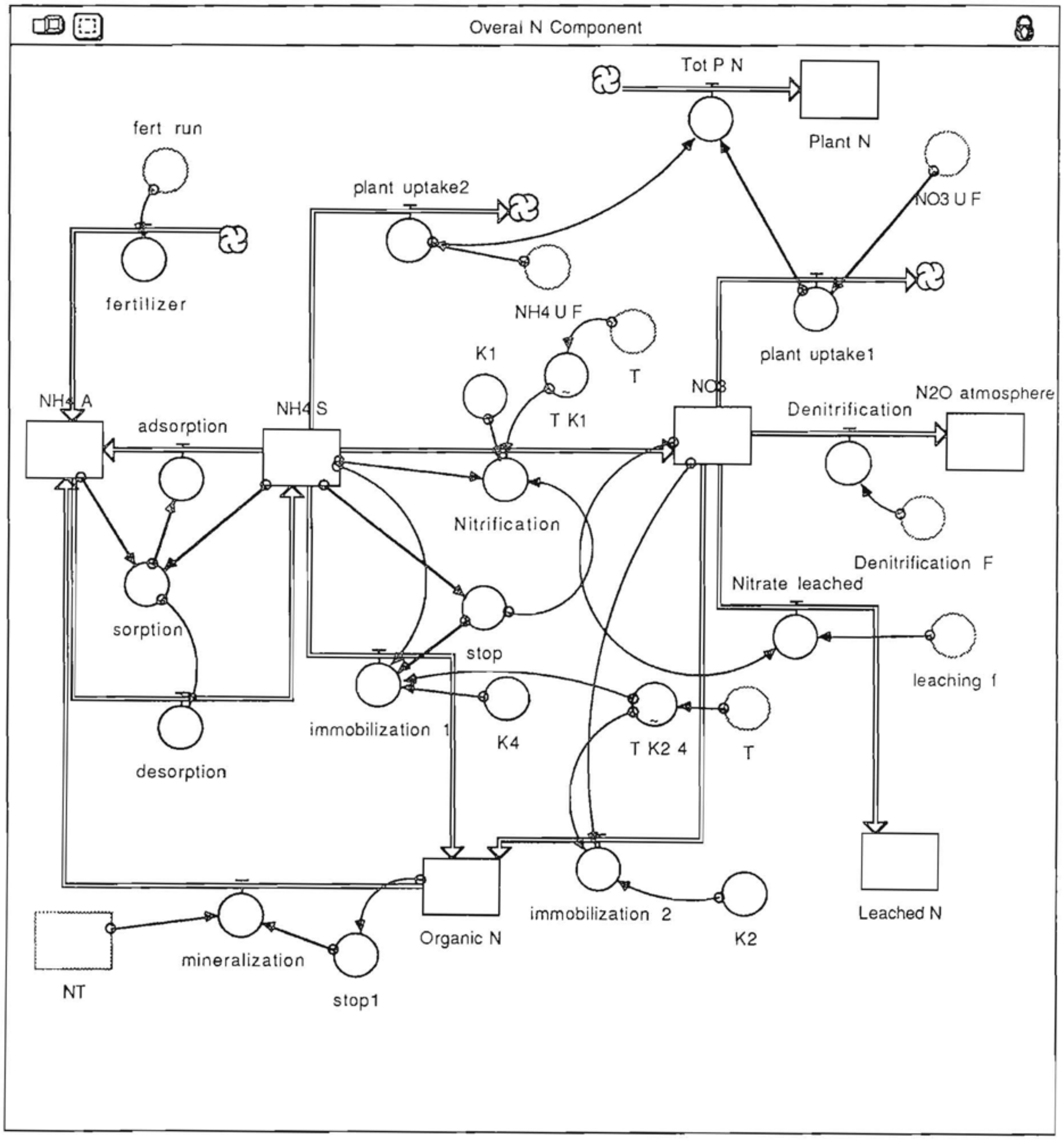


**Fig. 3. Schematic of the screen view of the overall N component of the N model. This section simulates the flow of N between N pools, as depicted in Fig. 1.**

through a dynamic interface. The beginning user needs only specify the conditions for a scenario to be simulated by entering appropriate values after clicking the mouse in the appropriate circle in the scenario section. The scenario section of the model (Table 1) contains converters that permit the user to make a series of choices pertaining to corn (*Zea mays* L.) production.

After choosing the desired condition from each section for a desired scenario, the user signals the computer to begin running the N cycle (solving the network of simultaneous linear equations as a function of time), and results for each time-step are displayed either as numerical values, as time-series graphs, or as animated icons on the screen.

## In-Depth

The second level (in-depth) was established so that students interested in acquiring a better understanding of particular segments of the N cycle can also see how the component was modeled and mathematically formulated. This level also includes specific literature citations from which model components were developed (e.g., Hagin et al., 1984; Reddy et al., 1980; Rolston et al., 1984; Stanford and Smith, 1972) embedded in the code for ready reference.

Table 1. Choices contained in converters in the scenario section of N model.

| Converter† | Choices |
|---|---|
| Rain | 1—Above average rainfall.<br>2—Average rainfall.<br>3—Below average season. |
| Temperature | 1—Average temperature.<br>2—Cool spring.<br>3—Warm spring and summer. |
| Fertilization | 0—No N fertilizer application.<br>1—168 kg N/ha application at planting.<br>2—168 kg N/ha split application. |
| Planting day | 1—15 April<br>2—1 May<br>3—15 May |
| Corn yield | Expected yield in kg/ha (140) |
| Soil type | 1—Sandy loam<br>2—Silty clay loam |

† Converters are model components as shown in Fig. 2.

## Advanced

The third level (advanced) allows for refinement of the model to reflect advancements in scientific understanding of certain aspects of the N cycle or inclusion of other processes that may play a significant role in the system. We do not wish to imply that our program is a complete rendition of the N cycle, but rather a learning tool for understanding the processes that are involved. Major components of the N cycle are included, but redefinition of processes already modeled or inclusion of additional processes by model users is encouraged as a means of furthering our understanding of the N cycle.

# Model Components

The simulation model can be divided into four major components, which operate codependently to perform the simulation. These components are: (i) scenario selection component, (ii) overall N component, (iii) N transformation component, and (iv) soil water component.

The scenario selection component provides the user with a series of choices that establish conditions for the model to simulate. The overall N component provides the general N cycle depicted in Fig. 1. The N transformation component provides regulation of N transformations and the soil water component provides simulation of weather conditions such as soil moisture. A typical example of the STELLA II screen depiction for this model is shown in Fig. 3.

## Scenario Selection Component

The scenario selection component consists of six different converters, each containing a series of choices (Table 1) that establish the parameters to be simulated. Each converter corresponds to a parameter or function definition statement in the model code, which has been preset to a default value. Each represents several lines of program code that provide the main computer program with example data that will subsequently be used in simulating actions of the N cycle. The user can choose a set of example data by simply typing a different number into the computer before beginning a simulation run. Default values for soil and weather conditions in the examples are based on conditions commonly found in Auburn, AL, and were generated using procedures described by Richardson (1985). The user is free to choose any desired combination of parameters from the scenario section for simulation. For example, a user choosing to adjust the *rain* section will be offered three choices for the rainfall distribution during the growing season: average, below average, and above average rainfall distribution. Selection of average will generate a rainfall pattern that is typical for the Auburn, AL, area and uses this to regulate input of rain into the soil water component of the model. Users with a preference for other geographic areas can substitute appropriate climatological parameters into the climate-generating program.

## Overall Nitrogen Component

The major components of the N cycle depicted in Fig. 1 are found in this section (Fig. 3). The concentrations of N in the various N pools are calculated in stocks contained in this portion of the model. The flow of N between the various N pools generally follows that depicted in Fig. 1, however, unlike the Fig. 1 schematic, both fertilizer $NH_4^+$ and mineralized $NH_4^+$ feed directly into the adsorbed $NH_4^+$ pool in the actual coding and operation of the model. This is based on an assumption that adsorption of $NH_4^+$ is practically instantaneous (compared with the 24-h time-step used by the model). If large amounts of $NH_4^+$ were suddenly added to the solution $NH_4^+$ compartment (for the duration of a full-day-long time-step), it would disrupt the equilibrium of many other reactions that are linked to the soluble $NH_4^+$ component.

Fertilizer N is added as anhydrous ammonia or $NH_4^+$ only. The $NH_4^+$ in solution can be immobilized, nitrified, absorbed, or taken up by plants. The immobilization and nitrification are regulated by constants, *K*, which depend on temperature and soil moisture availability. Soil N flows into the $NO_3^-$ pool as $NH_4^+$ is nitrified, where it can be leached, immobilized, denitrified, or taken up by plants. Immobilization of $NO_3^-$ is similar to $NH_4^+$ immobilization with a different *K* value regulation. Leaching is regulated through the soil water movement in the model. Plant uptake (called '*Tot P N*') in this section is a sum of the N from $NH_4^+$ and $NO_3^-$ removed from the soil N pools due to plant uptake.

The converters located in this component interact to regulate the flow of N between N pools. For example, the converter (*circle*) labeled *sorption* represents the Freundlich adsorption equation (Lyman, 1982) (Eq. [1]).

$$x/m = C\,K^{l/n} \quad [1]$$

where $x$ = the amount of chemical absorbed per mole ($m$), $C$ = the amount of chemical in solution (weight per unit soil volume), and $K^{l/n}$ = the adsorption coefficient. Arrows leading into the circle labeled *sorption* show that both $NH_4^+$ adsorbed on the soil exchange complex and $NH_4^+$ in soil solution will influence the calculation of $x/m$. Then, the adsorption isotherm, in turn, contributes to the calculation of both adsorption and desorption, indicated by the direction of arrows of the pipes connecting labeled stocks.

Persons wishing to examine the details of the underlying equations can see either the equations themselves or their numerical values by clicking the mouse button and requesting an on-screen display. Other users, such as those who are more concerned with model outcome than with its underlying causes, see only the display shown in Fig. 3 with its logical explanation of cause and effect. The auxiliary variables named *stop* and in the diagram check for negative values of $NH_4^+$, which could occur if the reaction(s) consumed all available substrate during a simulated time-step. Clearly, negative substrate values are meaningless, so the stop variables simply stop the reaction at this point. The effect is that of setting the equation equal to zero when the balance between the two rates are equal.

### Nitrogen Transformation Component

This component calculates complex factors that regulate N transformations or material flow in the overall soil N component of the model, such as denitrification, mineralization, and plant N uptake. Denitrification is based on $NO_3^-$ concentration, soil temperature, soil moisture, and the soluble C content of the soil. Soluble C is derived from the total soil organic matter content. The value for total organic matter, along with moisture and temperature values, are set by choices made in the initial *scenario* section of the model. Plant N uptake is based on an average N uptake curve for corn given by Ritchie et al. (1989). The total N removed by the plant is calculated based on estimated yield for corn (set in the scenario section of the model). The model removes equal amounts of N from the $NH_4^+$ pool and the $NO_3^-$ pool, as regulated by the plant uptake pattern for the given time of year. Other factors in the model regulate the amount of N removed from each pool as remaining N in each pool approaches zero.

### Soil Water Component

The soil water component tracks water movement in the soil, monitoring the various additions and removals by system constituents (rainfall, surface runoff, evapotranspiration, and leaching to groundwater). Addition of water to the system as rain will add weight to the soil (expressed as the sum of mineral, organic, and water components) and loss of water through evapotranspiration or leaching will subtract weight. The volumetric soil water content (*theta*) is computed directly from soil weight, and it regulates many other N transformation reactions in other portions of the model. Leaching rate is also computed in this section of the model, based on current saturation of the soil profile. When the soil profile is saturated, additional rainwater causes an equivalent volume of water to leach from the profile (*percolation*); whenever soil water content is below field capacity (*saturation value*), the profile must be fully recharged before water held in soil storage will leach below the rooting zone.

## DISCUSSION

Examples of simulation output are shown in Fig. 4 and 5. The main components of the N cycle (i.e., $NH_4^+$ absorbed, $NH_4^+$ in solution, and $NO_3^-$) are graphed as a function of time while the program is running. Stock variables (rectangles in the display screens shown in Fig. 3) and rates (valve symbols in Fig. 3) also are animated to display the current status of each variable during the actual running of the model. Numerical values can be displayed or stored in tabular form for later analysis of output data. The user is left to explore the outcome of their actions and, from noting model response, gain an intuitive understanding of how the system works.

Figures 4 and 5 show graphic results of changes over time for several N pools as affected by choices made in the scenario component of the model. The graphs shown in these figures are typical of the graph output found in the N model. For this example, only the soil type selection or the rainfall selection was changed. In the figures, graphs 1 and 2 represent silty clay loam, whereas graphs 3 and 4 represent a sandy loam soil. Likewise, graphs 1 and 3 represent above average rainfall, and graphs 2 and 4 represent below average rainfall. Comparison of the graphs produced from making one or more changes allowed in the scenario component shows the student how these changes affect the various components of the N cycle. Thus, the student becomes aware of the complexities of the N cycle and the intricacy of the system components and interactions with the soil environment.

In addition, alternative formulations of defining equations can also be explored; N will enter groundwater or be lost to the atmosphere only under certain conditions, and our model helps users define these conditions for their specific situations. The model provides the basic building blocks for computer modeling of the N cycle, so that further explorations of specific components can be explored. In this manner, the student can become aware of not only the intricacies of the N cycle but also take advantage of the merits of computer modeling of the N cycle without the burden of understanding the complexities of computer languages. With the use of this basic building block, the student is free (or can be assigned as a class project) to refine small portions of the N model to gain a better understanding of both the interactive nature of the soil environment and the computer modeling process itself.

Computer simulation models of complex systems can be helpful in understanding the system. Because of its importance in many aspects of agricultural production and environmental science, it is important that students and others concerned with these subjects understand the dynamics of the N cycle in the soil-plant system. This model provides a teaching tool to both explore the complexities of the N cycle and to gain an understanding of how simulation models can be used to provide the most precise picture of our present understanding of complex systems such as the N cycle. It is our belief that this model could be an excellent teaching tool and that implementation of this model into classroom or laboratory activities could provide students with greater appreciation and understanding of the N cycle.

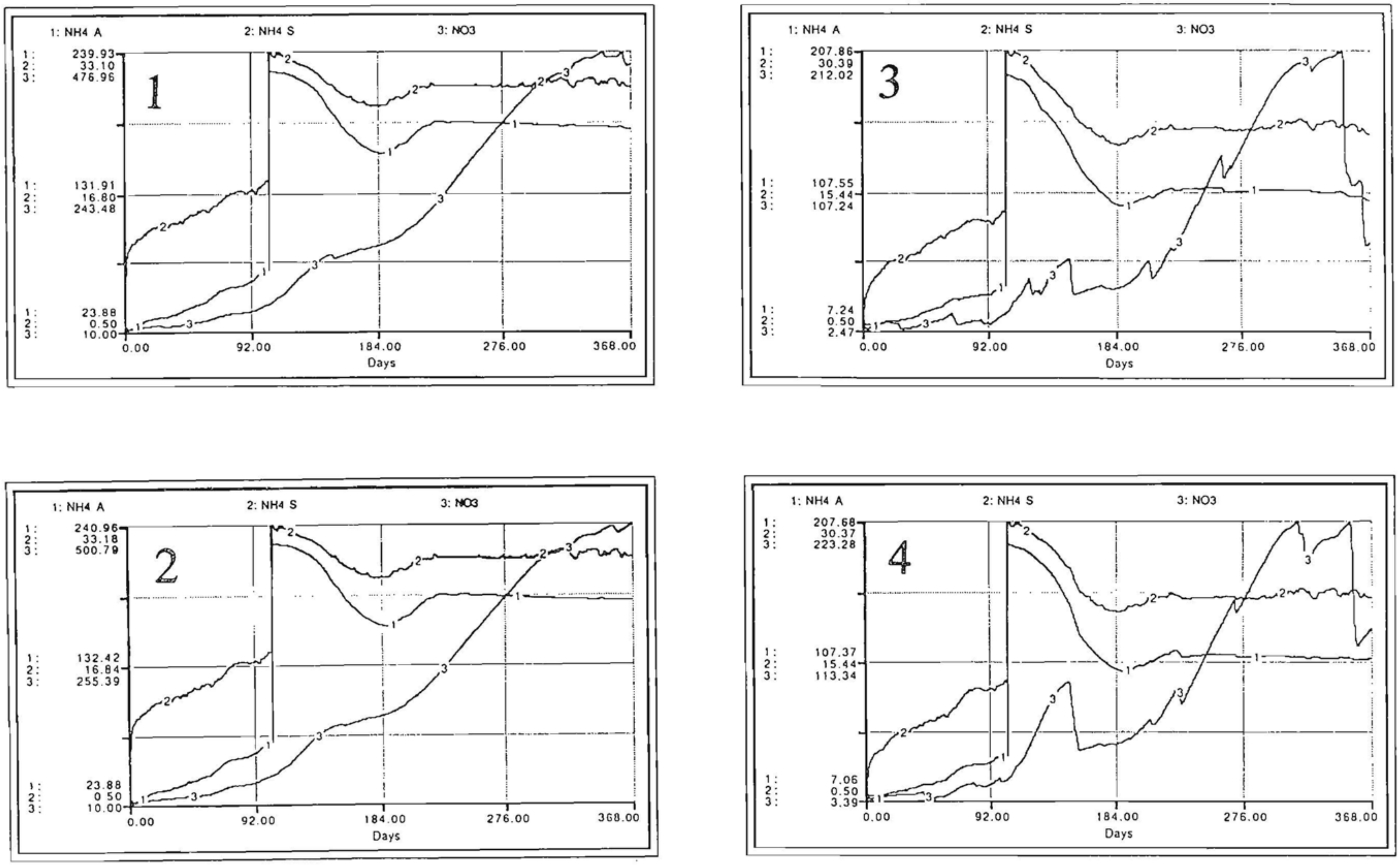


Fig. 4. Graphic results of changes over time of the $NH_4$-absorbed ($NH_4A$), $NH_4$-solution ($NH_4S$) and $NO_3$-N ($NO_3$) pools as affected by choices in the scenario section of the model.

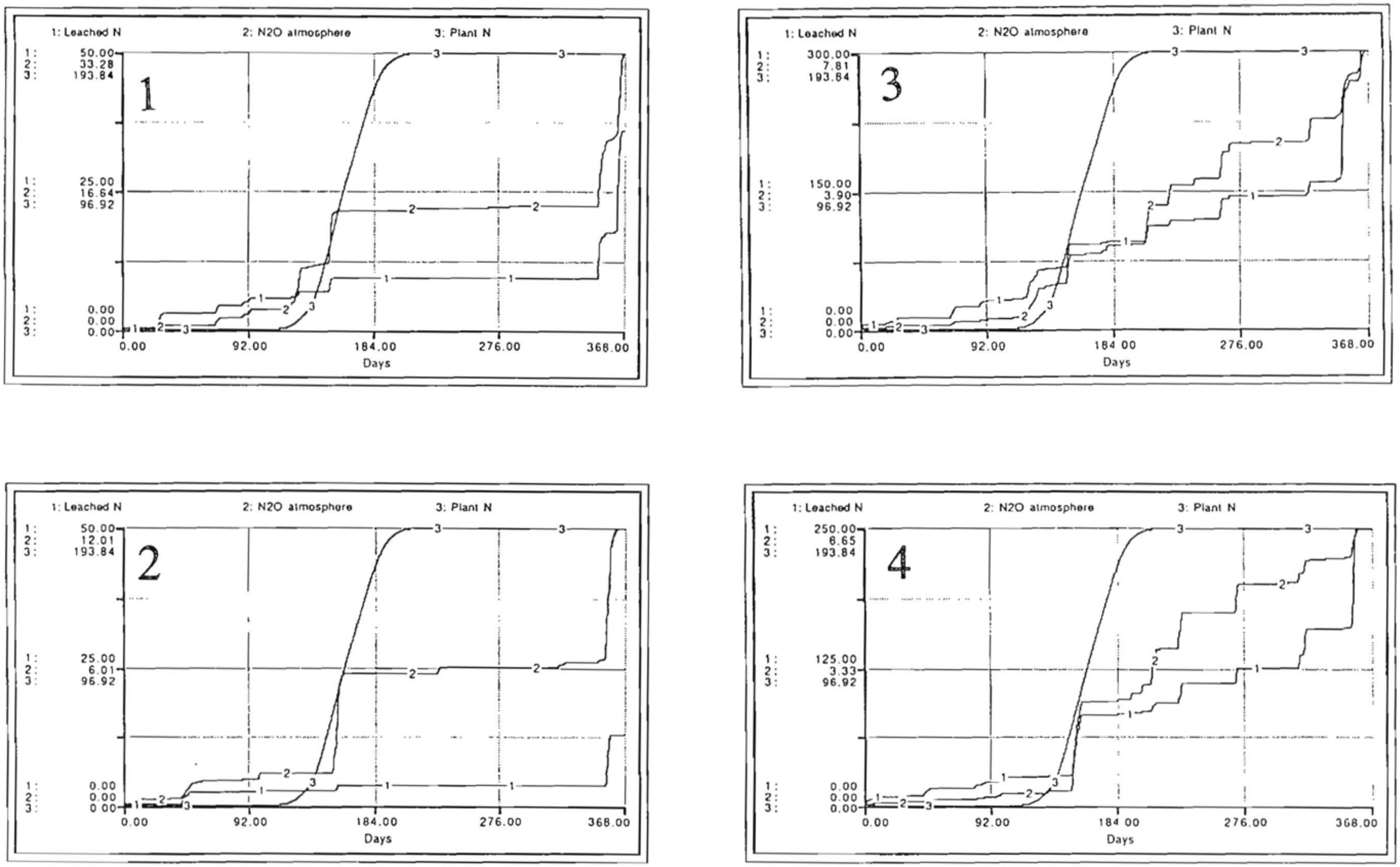


Fig. 5. Graphic results of changes over time of leached N, $N_2O/N_2$, and plant N uptake as affected by choices in the scenario section of the model.

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